

## Study guide: Time-dependent problems and variational forms

Hans Petter Langtangen<sup>1,2</sup>

Center for Biomedical Computing, Simula Research Laboratory<sup>1</sup>

Department of Informatics, University of Oslo<sup>2</sup>

Oct 29, 2015

## Time-dependent problems

- So far: used the finite element framework for discretizing in space
- What about  $u_t = u_{xx} + f$ ?
  - 1 Use finite differences in time to obtain a set of recursive spatial problems
  - 2 Solve the spatial problems by the finite element method

## Example: diffusion problem

$$\begin{aligned} \frac{\partial u}{\partial t} &= \alpha \nabla^2 u + f(\mathbf{x}, t), & \mathbf{x} \in \Omega, t \in (0, T] \\ u(\mathbf{x}, 0) &= l(\mathbf{x}), & \mathbf{x} \in \Omega \\ \frac{\partial u}{\partial n} &= 0, & \mathbf{x} \in \partial\Omega, t \in (0, T] \end{aligned}$$

## A Forward Euler scheme: ideas

$$[D_t^+ u = \alpha \nabla^2 u + f]^n, \quad n = 1, 2, \dots, N_t - 1$$

Solving wrt  $u^{n+1}$ :

$$u^{n+1} = u^n + \Delta t (\alpha \nabla^2 u^n + f(\mathbf{x}, t_n))$$

- $u^n = \sum_j c_j^n \psi_j \in V$ ,  $u^{n+1} = \sum_j c_j^{n+1} \psi_j \in V$
- Compute  $u^0$  from  $l$
- Compute  $u^{n+1}$  from  $u^n$  by solving the PDE for  $u^{n+1}$  at each time level

## A Forward Euler scheme: stages in the discretization

- $u_e(\mathbf{x}, t)$ : exact solution of the PDE problem
- $u_e^n(\mathbf{x})$ : exact solution of time-discrete problem (after applying a finite difference scheme in time)
- $u_e^n(\mathbf{x}) \approx u^n = \sum_{j \in \mathcal{I}_n} c_j^n \psi_j$  = solution of the time- and space-discrete problem (after applying a Galerkin method in space)

$$\frac{\partial u_e}{\partial t} = \alpha \nabla^2 u_e + f(\mathbf{x}, t)$$

$$u_e^{n+1} = u_e^n + \Delta t (\alpha \nabla^2 u_e^n + f(\mathbf{x}, t_n))$$

$$u_e^n \approx u^n = \sum_{j=0}^N c_j^n \psi_j(\mathbf{x}), \quad u_e^{n+1} \approx u^{n+1} = \sum_{j=0}^N c_j^{n+1} \psi_j(\mathbf{x})$$

$$R = u^{n+1} - u^n - \Delta t (\alpha \nabla^2 u^n + f(\mathbf{x}, t_n))$$

## A Forward Euler scheme: weighted residual (or Galerkin) principle

$$R = u^{n+1} - u^n - \Delta t (\alpha \nabla^2 u^n + f(\mathbf{x}, t_n))$$

The weighted residual principle:

$$\int_{\Omega} R w \, d\mathbf{x} = 0, \quad \forall w \in W$$

results in

$$\int_{\Omega} [u^{n+1} - u^n - \Delta t (\alpha \nabla^2 u^n + f(\mathbf{x}, t_n))] w \, d\mathbf{x} = 0, \quad \forall w \in W$$

Galerkin:  $W = V$ ,  $w = v$

## A Forward Euler scheme: integration by parts

Isolating the unknown  $u^{n+1}$  on the left-hand side:

$$\int_{\Omega} u^{n+1} \psi_i dx = \int_{\Omega} [u^n + \Delta t (\alpha \nabla^2 u^n + f(x, t_n))] \psi_i dx$$

Integration by parts of  $\int \alpha (\nabla^2 u^n) \psi_i dx$ :

$$\int_{\Omega} \alpha (\nabla^2 u^n) \psi_i dx = - \int_{\Omega} \alpha \nabla u^n \cdot \nabla \psi_i dx + \underbrace{\int_{\partial \Omega} \alpha \frac{\partial u^n}{\partial n} \psi_i dx}_{=0 \quad \leftarrow \quad \frac{\partial u^n}{\partial n} = 0}$$

Variational form:

$$\int_{\Omega} u^{n+1} \psi_i dx = \int_{\Omega} u^n \psi_i dx - \Delta t \int_{\Omega} \alpha \nabla u^n \cdot \nabla \psi_i dx + \Delta t \int_{\Omega} f^n \psi_i dx, \quad \forall \psi_i \in V$$

## New notation for the solution at the most recent time levels

- $u$  and  $u_i$ : the spatial unknown function to be computed
- $u_1$  and  $u_{-1}$ : the spatial function at the previous time level  $t - \Delta t$
- $u_2$  and  $u_{-2}$ : the spatial function at  $t - 2\Delta t$
- This new notation gives close correspondence between code and math

$$\int_{\Omega} uv dx = \int_{\Omega} u_1 v dx - \Delta t \int_{\Omega} \alpha \nabla u_1 \cdot \nabla v dx + \Delta t \int_{\Omega} f^n v dx$$

or shorter

$$(u, v) = (u_1, v) - \Delta t (\alpha \nabla u_1, \nabla v) + \Delta t (f^n, v)$$

## Deriving the linear systems

- $u = \sum_{j=0}^N c_j \psi_j(x)$
- $u_1 = \sum_{j=0}^N c_{1,j} \psi_j(x)$
- $\forall v \in V$ : for  $v = \psi_i$ ,  $i = 0, \dots, N$

Insert these in

$$(u, \psi_i) = (u_1, \psi_i) - \Delta t (\alpha \nabla u_1, \nabla \psi_i) + \Delta t (f^n, \psi_i)$$

and order terms as matrix-vector products ( $i = 0, \dots, N$ ):

$$\sum_{j=0}^N \underbrace{(\psi_i, \psi_j)}_{M_{i,j}} c_j = \sum_{j=0}^N \underbrace{(\psi_i, \psi_j)}_{M_{i,j}} c_{1,j} - \Delta t \sum_{j=0}^N \underbrace{(\nabla \psi_i, \alpha \nabla \psi_j)}_{K_{i,j}} c_{1,j} + \Delta t (f^n, \psi_i)$$

## Structure of the linear systems

$$Mc = Mc_1 - \Delta t Kc_1 + \Delta t f$$

$$\begin{aligned} M &= \{M_{i,j}\}, \quad M_{i,j} = (\psi_i, \psi_j), \quad i, j \in \mathcal{I}_s \\ K &= \{K_{i,j}\}, \quad K_{i,j} = (\nabla \psi_i, \alpha \nabla \psi_j), \quad i, j \in \mathcal{I}_s \\ f &= \{(f(x, t_n), \psi_i)\}_{i \in \mathcal{I}_s} \\ c &= \{c_i\}_{i \in \mathcal{I}_s} \\ c_1 &= \{c_{1,i}\}_{i \in \mathcal{I}_s} \end{aligned}$$

## Computational algorithm

- 1 Compute  $M$  and  $K$ .
- 2 Initialize  $u^0$  by either interpolation or projection
- 3 For  $n = 1, 2, \dots, N_t$ :
  - 1 compute  $b = Mc_1 - \Delta t Kc_1 + \Delta t f$
  - 2 solve  $Mc = b$
  - 3 set  $c_1 = c$

Initial condition:

- Either interpolation:  $c_{1,j} = l(x_j)$  (finite elements)
- Or projection: solve  $\sum_j M_{i,j} c_{1,j} = (l, \psi_i)$ ,  $i \in \mathcal{I}_s$

## Comparing P1 elements with the finite difference method: ideas

- P1 elements in 1D
- Uniform mesh on  $[0, L]$  with cell length  $h$
- No Dirichlet conditions:  $\psi_i = \varphi_i$ ,  $i = 0, \dots, N = N_n - 1$
- Have found formulas for  $M$  and  $K$  at the element level
- Have assembled the global matrices
- Have developed corresponding finite difference operator formulas
- $M$ :  $h[D_t^+(u + \frac{1}{6}h^2 D_x D_x u)]_i^n$
- $K$ :  $h[\alpha D_x D_x u]_i^n$

### Comparing P1 elements with the finite difference method; results

Diffusion equation with finite elements is equivalent to

$$[D_t^+(u + \frac{1}{6}h^2 D_x D_x u) = \alpha D_x D_x u + f]_i^n$$

Can lump the mass matrix by Trapezoidal integration and get the standard finite difference scheme

$$[D_t^+ u = \alpha D_x D_x u + f]_i^n$$

### Discretization in time by a Backward Euler scheme

Backward Euler scheme in time:

$$[D_t^- u = \alpha \nabla^2 u + f(\mathbf{x}, t)]^n$$

$$u_e^n - \Delta t (\alpha \nabla^2 u_e^n + f(\mathbf{x}, t_n)) = u_e^{n-1}$$

$$u_e^n \approx u^n = \sum_{j=0}^N c_j^n \psi_j(\mathbf{x}), \quad u_e^{n+1} \approx u^{n+1} = \sum_{j=0}^N c_j^{n+1} \psi_j(\mathbf{x})$$

### The variational form of the time-discrete problem

$$\int_{\Omega} (u^n v + \Delta t \alpha \nabla u^n \cdot \nabla v) \, dx = \int_{\Omega} u^{n-1} v \, dx + \Delta t \int_{\Omega} f^n v \, dx, \quad \forall v \in V$$

or

$$(u, v) + \Delta t (\alpha \nabla u, \nabla v) = (u_1, v) + \Delta t (f^n, \psi_i)$$

The linear system: insert  $u = \sum_j c_j \psi_j$  and  $u_1 = \sum_j c_{1,j} \psi_j$ ,

$$(M + \Delta t K)c = M c_1 + \Delta t f$$

### Calculations with P1 elements in 1D

Can interpret the resulting equation system as

$$[D_t^-(u + \frac{1}{6}h^2 D_x D_x u) = \alpha D_x D_x u + f]_i^n$$

Lumped mass matrix (by Trapezoidal integration) gives a standard finite difference method:

$$[D_t^- u = \alpha D_x D_x u + f]_i^n$$

### Dirichlet boundary conditions

Dirichlet condition at  $x = 0$  and Neumann condition at  $x = L$ :

$$\begin{aligned} u(\mathbf{x}, t) &= u_0(\mathbf{x}, t), & \mathbf{x} \in \partial\Omega_D \\ -\alpha \frac{\partial}{\partial n} u(\mathbf{x}, t) &= g(\mathbf{x}, t), & \mathbf{x} \in \partial\Omega_N \end{aligned}$$

Forward Euler in time, Galerkin's method, and integration by parts:

$$\int_{\Omega} u^{n+1} v \, dx = \int_{\Omega} (u^n - \Delta t \alpha \nabla u^n \cdot \nabla v) \, dx + \Delta t \int_{\Omega} f v \, dx - \Delta t \int_{\partial\Omega_N} g v \, ds,$$

Requirement:  $v = 0$  on  $\partial\Omega_D$

### Boundary function

$$u^n(\mathbf{x}) = u_0(\mathbf{x}, t_n) + \sum_{j \in \mathcal{I}_s} c_j^n \psi_j(\mathbf{x})$$

$$\begin{aligned} \sum_{j \in \mathcal{I}_s} \left( \int_{\Omega} \psi_i \psi_j \, dx \right) c_j^{n+1} &= \sum_{j \in \mathcal{I}_s} \left( \int_{\Omega} (\psi_i \psi_j - \Delta t \alpha \nabla \psi_j \cdot \nabla \psi_i) \, dx \right) c_j^n - \\ &\quad \int_{\Omega} (u_0(\mathbf{x}, t_{n+1}) - u_0(\mathbf{x}, t_n) + \Delta t \alpha \nabla u_0(\mathbf{x}, t_n) \cdot \nabla \psi_i) \, dx \\ &\quad + \Delta t \int_{\Omega} f \psi_i \, dx - \Delta t \int_{\partial\Omega_N} g \psi_i \, ds, \quad i \in \mathcal{I}_s \end{aligned}$$

### Finite element basis functions

- $B(\mathbf{x}, t_n) = \sum_{j \in I_b} U_j^n \varphi_j$
- $\psi_i = \varphi_{\nu(j)}$ ,  $j \in \mathcal{I}_s$
- $\nu(j)$ ,  $j \in \mathcal{I}_s$ , are the node numbers corresponding to all nodes without a Dirichlet condition

$$u^n = \sum_{j \in I_b} U_j^n \varphi_j + \sum_{j \in \mathcal{I}_s} c_{1,j} \varphi_{\nu(j)},$$

$$u^{n+1} = \sum_{j \in I_b} U_j^{n+1} \varphi_j + \sum_{j \in \mathcal{I}_s} c_{j,1} \varphi_{\nu(j)}$$

$$\begin{aligned} \sum_{j \in \mathcal{I}_s} \left( \int_{\Omega} \varphi_i \varphi_j \, dx \right) c_j &= \sum_{j \in \mathcal{I}_s} \left( \int_{\Omega} (\varphi_i \varphi_j - \Delta t \alpha \nabla \varphi_i \cdot \nabla \varphi_j) \, dx \right) c_{1,j} - \\ &\quad \sum_{j \in I_b} \int_{\Omega} (\varphi_i \varphi_j (U_j^{n+1} - U_j^n) + \Delta t \alpha \nabla \varphi_i \cdot \nabla \varphi_j U_j^n) \, dx \\ &\quad + \Delta t \int_{\Omega} f \varphi_i \, dx - \Delta t \int_{\partial \Omega_N} g \varphi_i \, ds, \quad i \in \mathcal{I}_s \end{aligned}$$

### Modification of the linear system; the raw system

- Drop boundary function
- Compute as if there are not Dirichlet conditions
- Modify the linear system to incorporate Dirichlet conditions
- $\mathcal{I}_s$  holds the indices of all nodes  $\{0, 1, \dots, N = N_n - 1\}$

$$\begin{aligned} \sum_{j \in \mathcal{I}_s} \underbrace{\left( \int_{\Omega} \varphi_i \varphi_j \, dx \right)}_{M_{i,j}} c_j &= \sum_{j \in \mathcal{I}_s} \underbrace{\left( \int_{\Omega} \varphi_i \varphi_j \, dx - \Delta t \int_{\Omega} \alpha \nabla \varphi_i \cdot \nabla \varphi_j \, dx \right)}_{M_{i,j}} c_{1,j} \\ &\quad + \underbrace{\Delta t \int_{\Omega} f \varphi_i \, dx - \Delta t \int_{\partial \Omega_N} g \varphi_i \, ds}_{f_i}, \quad i \in \mathcal{I}_s \end{aligned}$$

### Modification of the linear system; setting Dirichlet conditions

$$Mc = b, \quad b = Mc_1 - \Delta t K c_1 + \Delta t f$$

For each  $k$  where a Dirichlet condition applies,  $u(x_k, t_{n+1}) = U_k^{n+1}$ ,

- set row  $k$  in  $M$  to zero and 1 on the diagonal:  $M_{k,j} = 0$ ,  $j \in \mathcal{I}_s$ ,  $M_{k,k} = 1$
- $b_k = U_k^{n+1}$

Or apply the slightly more complicated modification which preserves symmetry of  $M$

### Modification of the linear system; Backward Euler example

Backward Euler discretization in time gives a more complicated coefficient matrix:

$$Ac = b, \quad A = M + \Delta t K, \quad b = Mc_1 + \Delta t f$$

- Set row  $k$  to zero and 1 on the diagonal:  $M_{k,j} = 0$ ,  $j \in \mathcal{I}_s$ ,  $M_{k,k} = 1$
- Set row  $k$  to zero:  $K_{k,j} = 0$ ,  $j \in \mathcal{I}_s$
- $b_k = U_k^{n+1}$

Observe:  $A_{k,k} = M_{k,k} + \Delta t K_{k,k} = 1 + 0$ , so  $c_k = U_k^{n+1}$

### Analysis of the discrete equations

The diffusion equation  $u_t = \alpha u_{xx}$  allows a (Fourier) wave component

$$u = A_e^n e^{ikx}, \quad A_e = e^{-\alpha k^2 \Delta t}$$

Numerical schemes often allow the similar solution

$$U_q^n = A^n e^{ikx}$$

- $A$ : amplification factor to be computed
- How good is this  $A$  compared to the exact one?

### Handy formulas

$$[D_t^+ A^n e^{ikq \Delta x}]^n = A^n e^{ikq \Delta x} \frac{A - 1}{\Delta t},$$

$$[D_t^- A^n e^{ikq \Delta x}]^n = A^n e^{ikq \Delta x} \frac{1 - A^{-1}}{\Delta t},$$

$$[D_t A^n e^{ikq \Delta x}]^{n+\frac{1}{2}} = A^{n+\frac{1}{2}} e^{ikq \Delta x} \frac{A^{\frac{1}{2}} - A^{-\frac{1}{2}}}{\Delta t} = A^n e^{ikq \Delta x} \frac{A - 1}{\Delta t},$$

$$[D_x D_x A^n e^{ikq \Delta x}]_q = -A^n \frac{4}{\Delta x^2} \sin^2 \left( \frac{k \Delta x}{2} \right)$$

### Amplification factor for the Forward Euler method; results

Introduce  $p = k\Delta x/2$  and  $C = \alpha\Delta t/\Delta x^2$ :

$$A = 1 - 4C \underbrace{\frac{\sin^2 p}{1 - \frac{2}{3}\sin^2 p}}_{\text{from } M}$$

(See notes for details)

Stability:  $|A| \leq 1$ :

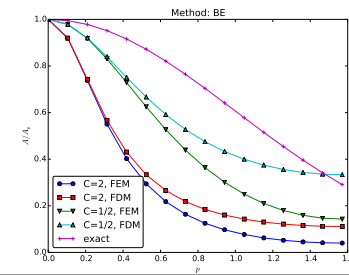
$$C \leq \frac{1}{6} \Rightarrow \Delta t \leq \frac{\Delta x^2}{6\alpha}$$

Finite differences:  $C \leq \frac{1}{2}$ , so finite elements give a *stricter* stability criterion for this PDE!

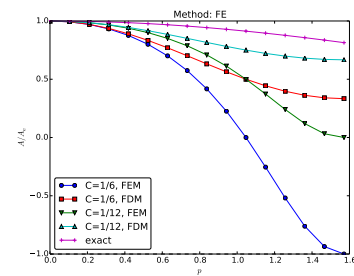
### Amplification factor for the Backward Euler method; results

Coarse meshes:

$$A = \left( 1 + 4C \frac{\sin^2 p}{1 + \frac{2}{3}\sin^2 p} \right)^{-1} \quad (\text{unconditionally stable})$$



### Amplification factors for smaller time steps; Forward Euler



### Amplification factors for smaller time steps; Backward Euler

